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Reliability of Polycrystalline HfO_2 thin films directly bonded to Si Substrates

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Abstract

The leakage current through polycrystalline HfO_2 films in submicron-sized capacitors was investigated, where we could measure the films' grain boundary length by AFM after electrode removal. We evaluated the current density per unit boundary length. Further, we demonstrated the advantage of polycrystalline films in terms of TDDB lifetime.

1. Introduction

Polycrystalline HfO_2 films have studied as candidates for high-k dielectrics to achieve EOT below 0.5nm [1] because of advantages, such as higher dielectric constant than amorphous films [2]. However, despite of its importance for device applications, the electrical characteristics of the polycrystalline films have not been revealed in detail. One of the information is that, for polycrystalline metal oxide thin films, the grain boundaries become leakage spots [3], and HfO_2 films are no exception [4]. In this work, quantitative analysis was done to evaluate the current density at grain boundaries and through grains. TDDB analysis was also done using small capacitors, with which we believe that the essence of reliability characteristics can be understood.

2. Experiment

A schematic cross section of the capacitor with the gate is shown in Fig. 1(a). After fabrication of the filed region (HfO_2/SiO_2-stacked area), 2.4 nm-thick amorphous HfO_2 films were directly deposited to Si substrates by ALD method. Then the films were crystallized by Rapid Thermal Crystallization anneal (RTC) method [1]. Some of the samples were annealed at 400°C in 10 Pa O_2 or forming gas. Then 30 μm x 30 μm sized Al gate electrodes were formed on top, and squared capacitors were fabricated. The length of a side of the capacitors was 500 nm. After measuring leakage current TDDB lifetime, the Al electrodes were removed and the topographic image of the HfO_2 surfaces was obtained to evaluate the lengths of the grain boundaries. Simple structured, as shown in Fig. 1(b), large scaled capacitors were also fabricated.

3. Results and discussion

Figure 2 shows *I-V* characteristics of the 16 capacitors of 500 nm in size. It is found that the leakage current is widely distributed among the capacitors. Figure 3 shows a typical topographic image of the HfO_2 surface obtained after Al removal. The grain boundaries are clearly visible in the image. We evaluated the lengths of grain boundaries for number of capacitors by taking AFM images, and the linear relation between boundary length and the leakage current is summarized in Fig. 4. The current was the values obtained at V_g=-0.5 V in this figure. The leakage current was attributed to TAT [5] (Trap-Assisted Tunneling), as seen in Fig. 5, and the evaluated trap levels were 0.92eV and 0.27eV, which are close to reported oxygen vacancy levels, 0.9eV and 0.3eV [6]. It was also found that the leakage current increased by forming gas annealing, and decreased by O_2 annealing, as seen in Fig. 6. The relation with the grain boundary length is again plotted in Fig. 7. It is interesting that the annealing only gives effects on the slope, and there is no significant change in the current value extrapolated at the boundary length of zero. The results demonstrate that oxygen-vacancy-related current paths exist at grain boundaries. According to the previous report that oxygen vacancy is hard to be generated in the crystalline grain than amorphous [7], it was concluded that oxygen vacancies move to grain boundaries during crystallization. Further, it seems that grain boundaries are thermally unstable compared to grains, then reaction during annealing was only seen in the boundaries.

The TDDB lifetime was also characterized. For large capacitors (30-μm squared), the lifetime is found to be overwhelmingly longer for amorphous films, and the lifetime distribution is more uniform for crystalline films, as shown in Fig. 8 and 9. However, both the lifetime and its uniformity are better for small capacitors (500-nm squared), as shown in Fig. 10. The results indicate that weak points which lead to breakdown are not randomly distributed in polycrystalline films. There seems to be some specific sites for weak point generation. It has not been clarified yet that the weak points are in the grains or at the boundaries. However, the results demonstrate the possibility that poly crystalline grains are intrinsically highly reliable than amorphous films.

4. Conclusions

By analyzing sub-micron scaled capacitors of polycrystalline HfO_2 films, it was demonstrated that the leakage current increased linearly with the length of grain boundaries. For application of polycrystalline HfO_2 films to devices, it is important to enlarge gains to minimize boundaries.

References
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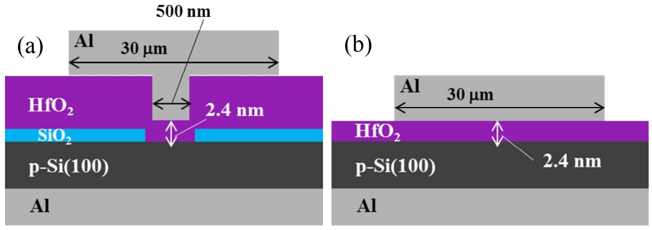

Fig. 1 MOS structure of (a) small and (b) large capacitctors.

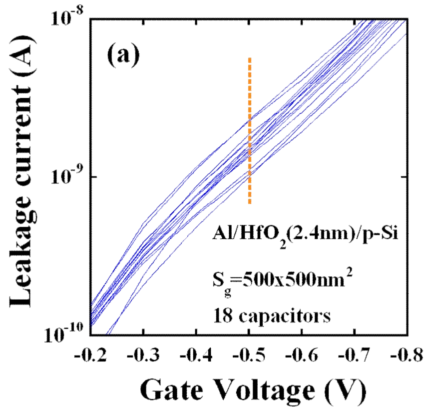

Fig. 2 I-V curves for small MOS capacitors.

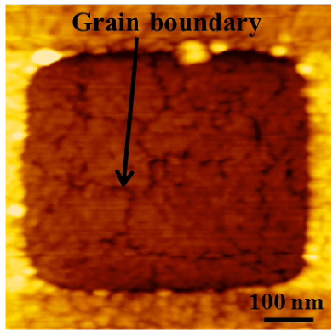

Fig. 3 AFM image of polycrystal-line HfO_2 surface obtained after Al removal from a small capacitor.

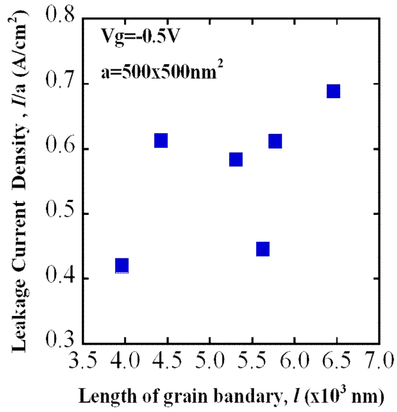

Fig. 4 Leakage current density for 6 capacitors vs. length of grain boundary.

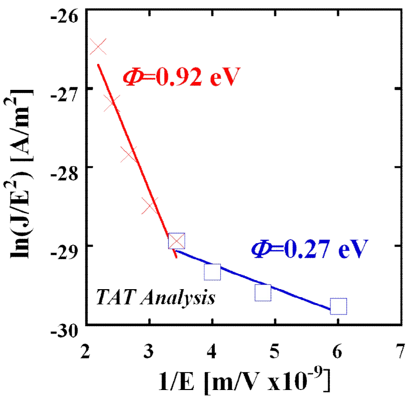

Fig. 5 TAT plots of the leakage current.

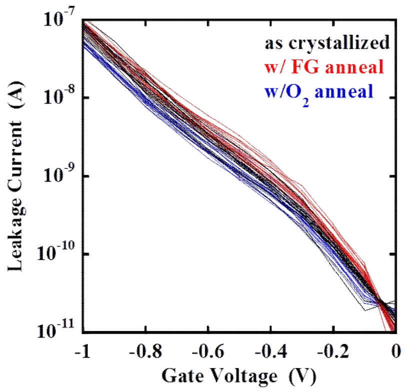

Fig. 6 I-V curves variation due to O_2 or FG anneal.

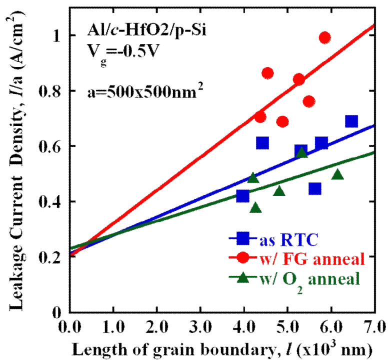

Fig. 7 Relation between current and length of the grain boundaries. Varia-tion due to annealing is also plotted.

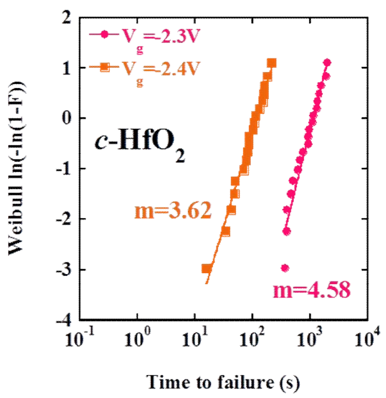

Fig. 8 TDDB lifetime for 30-μm squared capacitors with polycrystalline HfO_2 films. The stress voltages were -2.3 and -2.4 V.

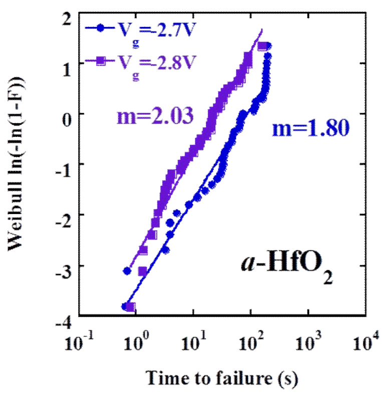

Fig. 9 TDDB lifetime for 30-μm squared capacitors with amorphous HfO_2 films. The stress voltages were -2.7 and -2.8 V.

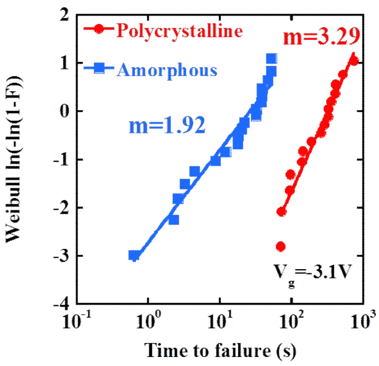

Fig. 10 TDDB lifetime for 500-nm squared capacitorsThe stress voltages were -3.1 V.